



## Environmental sustainability of bioethanol production from wheat straw in the UK

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### ABSTRACT

A UK-based environmental sustainability study on bioethanol production from wheat straw was conducted using a Life Cycle Assessment (LCA) approach. Five pathways with leading pretreatment technologies (dilute acid, steam explosion with and without catalyst, liquid hot water, and wet oxidation) were modelled using process simulation software AspenPlus™, and their advantages and disadvantages were evaluated from an environmental perspective. In a contribution analysis of the environmental profiles for the near-term prospective scenarios, results indicated that the enzyme is a main contributor in all pathways. In addition to enzyme production, acid catalyst and base for its subsequent neutralisation also cause significant environmental burdens for dilute acid and steam explosion with catalyst pathways. By comparing the five wheat straw production pathways with petrol, it was suggested that those using pretreatment with steam explosion, liquid hot water and wet oxidation can be environmentally favourable over petrol. However, a sensitivity analysis conducted by expanding the ethanol system boundary to include the consequential effects of removing wheat straw from the field, suggested an increase in the overall environmental burdens of ethanol life cycles but certain wheat straw ethanol pathway (i.e. with steam explosion pretreatment) still remain environmentally favourable over petrol.

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**Abbreviations:** AD, anaerobic digestion; GHG, greenhouse gas; ADP, abiotic resources depletion potential; HTP, human toxicity potential; AP, acidification potential; LCA, life cycle assessment; CHP, combine heat and power; LCIA, life cycle impact assessment; CFC-<sup>11</sup>, trichlorofluoromethane; LHW, liquid hot water; COD, chemical oxygen demand; ODP, Ozone layer depletion potential; DA, dilute acid; POCP, photochemical-oxidants creation potential; DB, dichlorobenzene; SE, steam explosion; EP, eutrophication potential; SEAC, steam explosion with acid catalyst; FAETP, freshwater aquatic ecotoxicity potential; TEP, terrestrial ecotoxicity potential; FFV, flexible-fuel vehicle; WO, wet oxidation; FPU, filter paper unit; WWT, wastewater treatment; gwp<sub>100</sub>, global warming potential (100 year horizon); VOC, volatile organic compounds

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## 1. Introduction

Biofuels have been recognised to be an alternative transport fuel to gasoline for decades and can be produced from a variety of sources including sugars, plant oils and lignocellulosic biomass. Agricultural wastes such as corn stover, wheat straw and sugarcane bagasse are becoming attractive feedstocks for bioethanol production since their utilisation is not competitive with food.

As one of the major crops in the UK, wheat is cultivated in many parts of the country [1]. The UK annual wheat straw yield has been estimated to be between 8 and 10 million tonnes [2]. In recent years, the market price of wheat straw has varied from approximately £25 per tonne in 2000 to £52 per tonne in 2010 [3]. However, due to rising gasoline prices and particularly the availability and relatively low cost of wheat straw compared with other lignocellulosic biomass, it serves as a potentially attractive feedstock for producing bioethanol.

Currently, several biorefineries in Europe utilising wheat straw as a feedstock to produce bioethanol have progressed to demonstration scale. Inbicon in Denmark produces 4300 t of bioethanol and also 11.1 thousand tonnes of molasses (65% dry matter) from 30,000 t wheat straw per year. Abengoa in Spain is processing wheat straw at the rate of 70 t per day, and produces over 5 million litres of ethanol per year. Süd-Chemie AG in Germany has started construction for a plant which will produce up to 1000 t of ethanol per year from wheat straw. Outside the EU, Iogen in Canada is also operating an ethanol biorefinery with wheat straw as its primary feedstock [4]. These established biorefineries suggest that bioethanol production from wheat straw is viewed as a potentially economically attractive pathway.

From an environmental point of view, the greenhouse gas (GHG) emission reduction target for the EU is 20% by 2020 (from 1990 levels), and for the UK it is 34% [5]. Therefore, timely environmental assessments in combination with economic analyses, on the potential of second generation (2G) bioethanol from lignocellulosic resources are required to assist policy making. There have been numerous studies on LCA of bioethanol from different biomass sources, such as corn stover [6,7], willow [8], switchgrass [9,10], miscanthus [10] and sugarcane [7,11]. Most of these focus on GHG emissions rather than a broad range of impact categories in their life cycle assessment and report example GHG emissions ranging from 7 g CO<sub>2</sub> eq./MJ for switchgrass derived ethanol [10] to 21 g CO<sub>2</sub> eq./MJ for sugarcane ethanol in Wang et al. study whilst 21 g CO<sub>2</sub> eq./MJ in Seabra et al.'s study [11]. The variations are mainly due to aspects of the methodologies applied and to differences in the technologies and data for the agricultural sector, bioethanol conversion technologies. By comparing bioethanol derived from such lignocellulosic biomass sources with the conventional fuel in some of these studies, GHG emissions savings against gasoline are found between 44% and 95% [7,12].

Review of the literature as summarised above indicates that there is currently relatively little research focused on assessing the 'well-to-wheel' environmental profile with full impact categories of wheat straw-derived bioethanol. Two comprehensive reviews have been published recently by Cherubini et al. [13] and Singh et al. [14] including the updated developments and challenges on the environmental sustainability assessment of bioenergy/bioethanol. It has been suggested that LCA is an appropriate approach to evaluate the potential use of lignocellulosic feedstocks in bioethanol production, screen new technologies, and to identify the main drivers of the environmental profile of bioethanol, thereby indicating priority areas for potential improvements [15–18]. However, there is an ongoing debate regarding the potential effects caused by the removal of agricultural residues.

Except for a few literature reports [19,20], the effects caused by wheat straw removal for bioethanol production purposes are neglected in most bioethanol LCA studies. Removal of wheat straw rather than ploughing back to the field may raise several concerns: (1) decreasing the soil quality which leads to additional synthetic fertiliser applied to balance the nutrients removed with the straw, (2) increasing field emissions due to applying additional fertiliser, and (3) decreasing soil organic carbon stock which leads to a loss of carbon as CO<sub>2</sub> to atmosphere. These effects caused by wheat straw removal on ethanol life cycles and comparison results with petrol are discussed thoroughly in this study.

In our previous study, the economic feasibility for several cases of bioethanol production at industrial scale from wheat straw using different 'state-of-the-art' pretreatment technologies (i.e. steam explosion with and without acid catalyst, liquid hot water, dilute acid and wet oxidation) have been conducted [21]. It was found that bioethanol production with steam explosion or liquid hot water, with a production cost at £0.28/L, can be economically competitive with petrol in a prospective scenario with a reduced enzyme loading [21]. It also indicated that policy support in the form of tax exemptions and the access to the wheat straw prices of £35/tonne or lower could significantly enhance competitiveness of bioethanol with petrol. In this study, the environmental profiles of these cases defined above are assessed using an LCA approach with many impact categories considered, and are then compared with the conventional transportation fuel petrol.

## 2. Methodology

LCA is a method assessing the environmental impacts of a product through its life cycle from the raw material acquisition and production, transportation to end-use and disposal. The LCA study was conducted with regard to ISO 140440 and its related standards [22]. With regards to the Life cycle impact assessment (LCIA), the characterisation model CML baseline 2000 v2.05 incorporated in software Simapro v7.3 was applied [23].

## 2.1. Scope of study and functional unit

This LCA study had two aims: (1) assessing the environmental profile of bioethanol produced from wheat straw using different 'state-of-the-art' pretreatment technologies through its 'well-to-wheel' life cycle; and (2) comparing bioethanol (E100) pathways with conventional petrol. Accordingly, the functional unit is defined as '*to drive 1 km in a Flexible-fuel vehicle (FFV)*'. In the comparison, the amount of fuel required to drive a FFV for 1 km was calculated as

**Table 1**  
Inventory data for inputs of wheat cultivation and harvest [33].

|  | Left in the field | Removed |
|--|-------------------|---------|
| <b>Fertilisers</b>                                     |                   |         |
| N fertiliser (as N), kg/ha                             | 185               | 253     |
| P fertiliser (as P), kg/ha                             | 41                | 164     |
| K fertiliser (as K), kg/ha                             | 46                | 53      |
| <b>Other inputs</b>                                    |                   |         |
| Diesel, l/ha   | 140               |         |
| Pesticides, kg/ha                                      | 2                 |         |
| Seed material, kg/ha                                   | 185               |         |
| Transportation for fertiliser, seed and pesticides, km | 100               |         |
| Transportation for wheat straw, km                     | 100               |         |

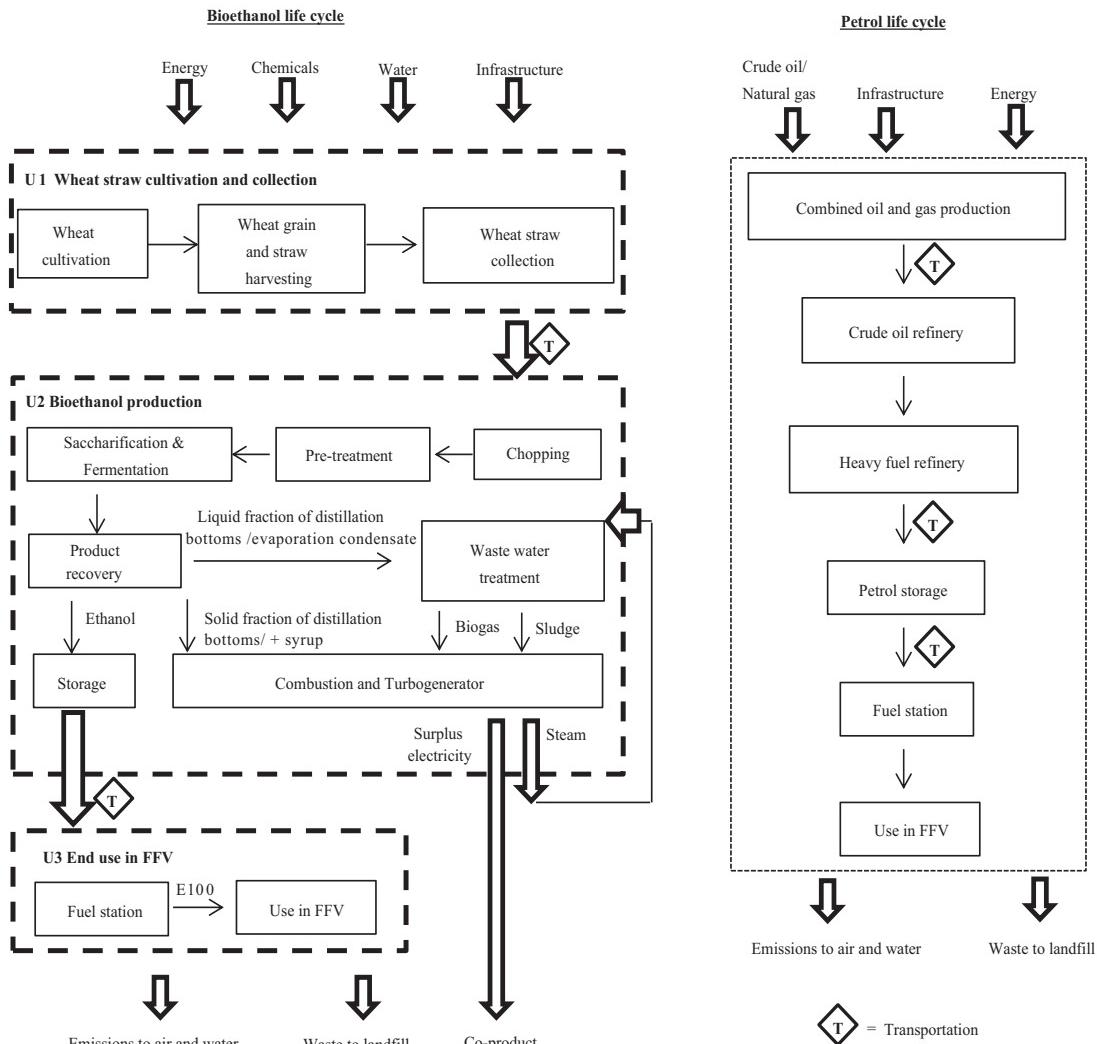
114 g for E100 and 70 g for petrol according to the assumed engine efficiency (0.32 km/MJ) and their respective energy contents (27.4 MJ/kg bioethanol and 44.7 MJ/kg petrol) [24].

## 2.2. System boundary

The original system boundaries for the bioethanol and petrol systems are shown in Fig. 1. In the bioethanol system, unit processes included (1) wheat straw cultivation and collection in the field (U1), (2) conversion of wheat straw to bioethanol and by-products (U2), (3) distribution of bioethanol to retail fuelling station and use of E100 in a FFV (U3). The petrol system includes the petrol production, distribution and its end use. When the sensitivity analysis on system boundary is studied, the expanded bioethanol system is described in Section 2.6.

## 2.3. Inventory analysis

In addition to literature reviews, computer models and supplier questionnaires were applied to develop LCA inventories in this study. The inventory data collection methods vary with the unit processes. For instance, inventory data for enzyme production were collected via questionnaires. Mass and energy balance data for bioethanol production process were obtained from computer



**Fig. 1.** System boundaries for bioethanol and petrol systems.

models (AspenPlus™) using data derived from literature reviews as the model inputs. Inventories for other input production such as wheat straw, petrol, chemicals, fertilisers and energy and for infrastructure was from Ecoinvent database v2.2 [25]. Inventories for output such as emission factors for agricultural field emission, fuel combustion in road transport and field operation were derived from the IPCC approach [26] and 2009 EMEP-EEA Guidebook [27].

### 2.3.1. Bioethanol system unit process – U1 wheat straw cultivation and collection

The average yield and price of wheat grain (with 16% water content) are 7.8 t/ha and 133 £/tonne (time period: 2007–2011) [28] while those for wheat straw are 3.2 t/ha and 52 £/tonne [3]. The wheat cultivation process includes several steps: ploughing, drilling, fertiliser spreading, pesticides application, combined harvesting and baling of wheat straw. The inventory data for inputs of wheat straw cultivation and collection are summarised in Table 1. Two sets of fertiliser usage data are presented: (1) wheat straw is left in the field, and (2) wheat straw is removed. The amount of additional fertiliser required to balance nutrients removed with wheat straw at different proportions are calculated accordingly. Emission factors for GHGs and other emissions due to diesel combustion during field operations were adopted from IPCC and EMEP-EEA, respectively [27,29]. Direct and indirect emissions of nitrous oxide ( $N_2O$ ) were calculated according to IPCC methods [30]. Phosphorous (P) and nitrogen (N) leaching to soil were estimated to be 1.5 kg/ha and 2.0 kg/ha based on Williams et al. [31]. The inventory data for fertiliser and other chemicals produced were from Ecoinvent v2.2 database research report [32].

### 2.3.2. Bioethanol system unit process—U2 bioethanol production from wheat straw

**2.3.2.1. Process design.** The composition of wheat straw, the pretreatment parameters and the results from subsequent enzymatic saccharification are derived from research literature [34,35]. Wheat straw, with a moisture content of 6.5% (w/w), contains 34.6% glucan, 21.1% xylan, 2.3% arabinan, 0.9% galactan, 18.0% lignin, 2.2% acetyl groups, 5.6% ash and 15.4% extractives (w/w on a dry basis).

The process design configuration (Fig. 2) was developed based on the NREL corn stover-to-bioethanol model [36] with

modifications according to different pretreatments applied. The pretreatment modelled was steam explosion with and without acid catalyst, dilute acid, liquid hot water and wet oxidation. The conditions of these pretreatments, results for the subsequent enzymatic hydrolysis and assumptions are described in the following subsection

The plant is designed to process 2000 dry metric tonnes of wheat straw per day. In Area A, wheat straw is bulk delivered to the bioethanol plant and is unwrapped, washed, milled and conveyed to Area B where pretreatment is performed with a total solids loading of 30% (w/w). The treated wheat straw is sent to separate hydrolysis and fermentation (Area C) where polysaccharides are hydrolysed to C5 and C6 monomer sugars which are both fermented to ethanol by the bacterium *Zymomonas mobilis*. Enzymatic saccharification is carried out at 50 °C for 72 h and fermentation operates at 32 °C for 36 h. Nutrient loadings and fermentation sugar conversion efficiencies (95% for glucose, 85% for xylose and arabinose) are adopted from the NREL process [36]. In saccharification, a commercial enzyme cocktail Cellic Ctec with an enzyme activity of 120 FPU/ml is assumed to be used at a relatively low enzyme loading (e.g. 10 FPU/g glucan) that is expected to be achievable in the near-term in industry scale.

Detailed design for Area B (pretreatment) and Area C (saccharification & fermentation) are presented as follows in Table 2 and in Fig. 3.

- Steam explosion without catalyst (SE):** wheat straw is mixed with process water recycled from wastewater treatment (WWT) (Area E) and heated up to 100 °C by high pressure steam (13 atm), and then heated to 180 °C by high pressure steam and maintained for 10 min before a sudden pressure release by sending the flow to a blowdown tank which vaporises acetic acid etc. [35].
- Steam explosion with acid catalyst (SEAC):** it is similar to SE but includes addition of dilute sulphuric acid at a concentration of 0.9% (w/w). After the blowdown tank, the flow is sent to a conditioning tank where ammonia is added to neutralise the hydrolysate to a suitable pH for saccharification [35].
- Dilute acid (DA):** the pretreatment operates with sulphuric acid (2% w/v) for 90 min at a temperature of 121 °C. Similar to SEAC, blowdown and conditioning tanks are required [37].

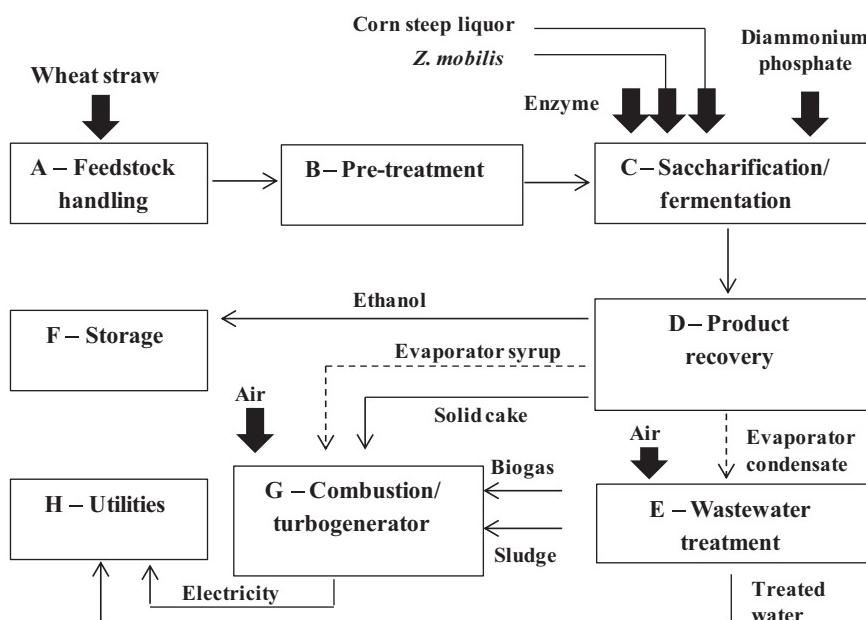


Fig. 2. A schematic diagram of the wheat straw-to-bioethanol process (streams shown in dashed lines vary in cases depending on process design differences in Area D).

**Table 2**

A summary of conditions and results for the selected pretreatment and enzymatic saccharification processes.

| Pretreatment method                     | Liquid hot water (LHW)                               | Steam explosion without catalyst (SE) | Steam explosion with H <sub>2</sub> SO <sub>4</sub> catalyst (SEAC) | Dilute acid (DA)  | Wet oxidation (WO)                       |
|---|--|---------------------------------------|---|---|--|
| Pretreatment conditions                 | 188 °C, 40 min                                       | 180 °C, 10 min                        | 180 °C, 10 min, 0.9% (w/w) H <sub>2</sub> SO <sub>4</sub>           | 121 °C, 90 min, 2% (w/v) H <sub>2</sub> SO <sub>4</sub> | 180 °C, 15 min, O <sub>2</sub> at 12 bar |
| Pretreatment reactions                  | Fraction of reactant converted to product            |                                       |   |   |  |
| Glucan + H <sub>2</sub> O → Glucose     | 0%   | 10%                                   | 10%   | 12%   | 1.2%                                     |
| Glucan → HMF + H <sub>2</sub> O         | NA <sup>a</sup>                                      | 1.5%                                  | 0.15%   | 2.7%  | NA                                       |
| Xylan + H <sub>2</sub> O → Xylose       | 91%  | 95%                                   | 82%   | 85%   | 7.1%                                     |
| Xylan → Furfural + 2 H <sub>2</sub> O   | NA   | 0.35%                                 | 0.05%   | 0.2%  | 1.2%                                     |
| Arabinan + H <sub>2</sub> O → Arabinose | NA   | 94%                                   | 90%   | 100%  | NA                                       |
| Galactan + H <sub>2</sub> O → Galactose | NA   | 100%                                  | 100%  | NA  | NA                                       |
| Lignin → Soluble lignin                 | 19%  | 18%                                   | 32%   | 16%   | NA                                       |
| Enzymatic saccharification results      | 76.3% glucose yield, 20.5% xylose yield <sup>b</sup> | 60% glucose yield                     | 80% glucose yield   | 62.2% glucose yield, 73.9% xylose yield                 | 56% glucose yield, 65% xylose yield      |
| References                              | [34]   | [35]                                  | [35]  | [37]  | [38]                                     |

<sup>a</sup> NA=Data is not reported.

<sup>b</sup> Sugar yield is defined as the proportion of polysaccharides converted to monomeric sugars.

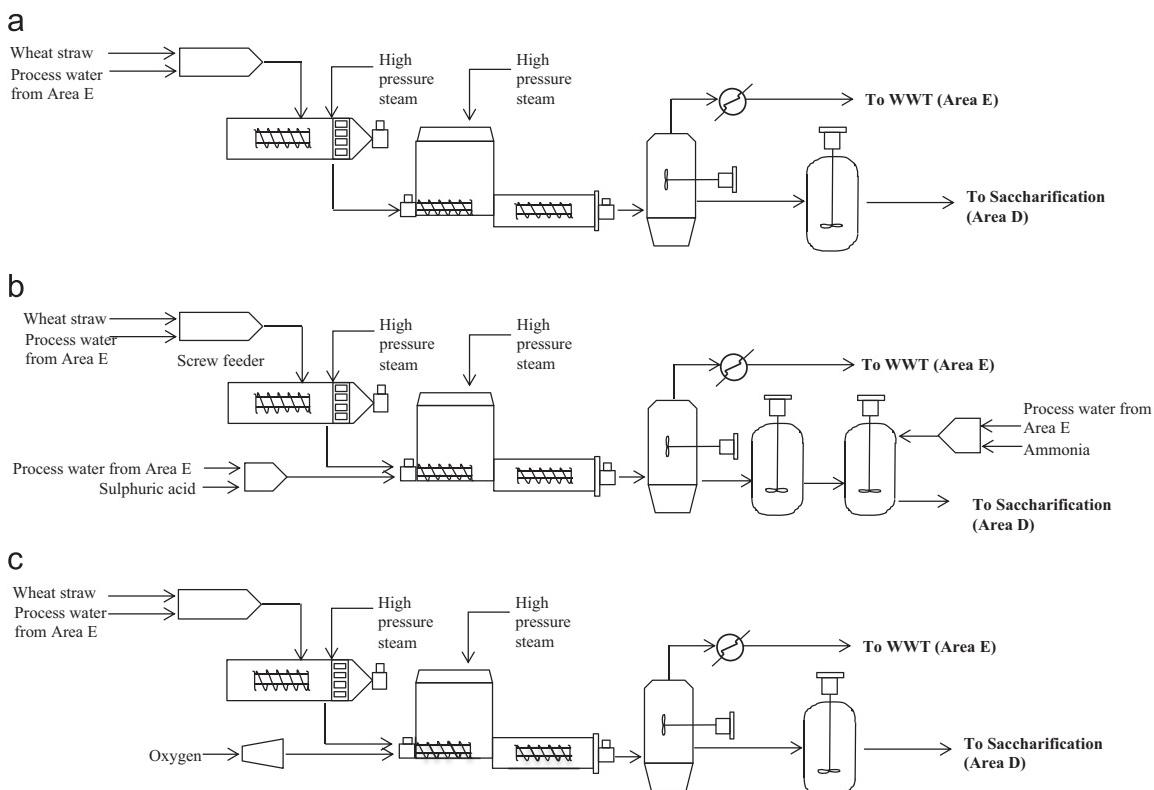


Fig. 3. Process design of five pretreatments in Area B ((a) for SE and LHW; (b) for DA and SEAC; and (c) for WO).

- d. *Liquid hot water (LHW)*: wheat straw is mixed with water and pre-heated to 100 °C before holding at 188 °C for 40 min [34].
- e. *Wet oxidation (WO)*: compressed O<sub>2</sub> at 12 bar is injected into the pre-heated (100 °C) mixture of wheat straw and water before being maintained at 180 °C for 15 min [38].

The fermentation beer from Area C is fed to Area D where ethanol is purified to 99.6% through distillation, rectification and molecular sieve adsorption. There are two options to deal with the distillation

bottoms which is determined by the type of pretreatment process selected: (1) a series of evaporators can concentrate the soluble organics as a syrup which is then fed to the combustor (Area G) for heat generation; or (2) a press filter can separate the solids which are sent to the combustor and the liquor is sent to wastewater treatment (Area E). In pretreatments where sulphuric acid is used as a catalyst i.e. SEAC and DA, ammonium sulphate generated as a result of acid neutralisation with ammonia becomes concentrated in the evaporator system used in option (1) and presents a fouling risk in

**Table 3**

Inventory data for five wheat straw-to-bioethanol cases.

|  | DA      | SEAC    | SE      | LHW     | WO      |
|--|---------|---------|---------|---------|---------|
| <b>Input</b>                             |         |         |         |         |         |
| Wheat straw, dry, kg/hr                  | 83,333  | 83,333  | 83,333  | 83,333  | 83,333  |
| Well water, kg/hr                        | 270,577 | 191,313 | 301,174 | 289,435 | 311,406 |
| Enzyme, kg/hr                            | 3973    | 3665    | 3644    | 4260    | 3790    |
| Sulphuric acid ( $H_2SO_4$ ), kg/hr      | 5781    | 2867    | —       | —       | —       |
| Corn steep liquor (CSL), kg/hr           | 1175    | 1176    | 1181    | 1175    | 1170    |
| Diammonium phosphate (DAP), kg/hr        | 156     | 156     | 156     | 156     | 155     |
| Ammonia, kg/hr                           | 2594    | 1528    | —       | —       | —       |
| NaOH, 50% in $H_2O$ <sup>a</sup> , kg/hr | 6124    | 3645    | —       | —       | —       |
| Lime, kg/hr                              | 6549    | 1451    | —       | —       | —       |
| <b>Output</b>                            |         |         |         |         |         |
| Bioethanol, kg/hr                        | 18,838  | 20,927  | 18,368  | 19,517  | 17,105  |
| Surplus electricity, MW                  | 13.6    | 1.6     | 25.8    | 19.6    | 26.4    |
| <b>Emissions</b>                         |         |         |         |         |         |
| $CO_2$ , kg/L bioethanol                 | 4.46    | 3.76    | 4.89    | 4.52    | 4.60    |
| $NO_x$ , kg/L bioethanol                 | 1.21E−3 | 9.47E−4 | 1.75E−3 | 1.27E−3 | 2.07E−3 |
| $CH_4$ , kg/L bioethanol                 | 4.45E−3 | 4.78E−3 | 5.18E−4 | 4.76E−4 | 6.98E−4 |
| $CO$ , kg/L bioethanol                   | 1.21E−3 | 9.47E−4 | 1.75E−3 | 1.27E−3 | 2.07E−3 |
| $SO_2$ , kg/L bioethanol                 | 3.07E−3 | 3.46E−3 | 1.96E−3 | 2.01E−3 | 1.18E−3 |
| $H_2SO_4$ , kg/L bioethanol              | 5.95E−4 | 6.69E−4 | 3.79E−4 | 3.89E−4 | 2.28E−4 |
| Ethanol, kg/L bioethanol                 | 1.27E−4 | 2.22E−4 | 1.35E−4 | 1.37E−4 | 1.16E−4 |
| <b>Waste</b>                             |         |         |         |         |         |
| Combustion bottom (kg/hr)                | 5483    | 5110    | 4841    | 4843    | 4900    |
| Gypsum (kg/hr)                           | 7369    | 3006    | —       | —       | —       |

<sup>a</sup> WWT chemical used in reverse osmosis membrane system for salt removal.

the combustion system [36]. Therefore, option (2) is employed with SEAC and DA pretreatment processes, pretreatment while option (1) is applied to SE, WO and LHW pretreatment processes.

WWT (Area E), including anaerobic digestion (AD) and aerobic digestion, treats used water and recycles it within the system. In AD, 91% of organic matter is converted into biogas and sludge. The biogas with a composition of 51%  $CH_4$ /49%  $CO_2$  (dry molar basis) is produced at a yield of 228 g biogas/kg COD (chemical oxygen demand) removed. The treated water is further cleaned in aerobic digestion where 96% of the remaining soluble organic matter is removed. In the SEAC and DA pretreatment processes, the cleaned water is sent to a reverse osmosis membrane system for salt removal (sodium nitrate) which is modelled as a brine waste for landfill disposal.

Solid cake from the distillation bottoms combined with the concentrated syrup from evaporators (where applicable), and biogas and sludge from WWT are fed to the Combined Heat and Power (CHP) generation system in Area G. High pressure (13 atm) and Medium pressure (9.5 atm) steam from the turbine is extracted, and generated electricity is used to supply the process requirement. Excess electricity is sold to the National Grid as a co-product credit. For the pretreatment processes involving acid (SEAC and DA), the flue gas released from the combustor requires desulphurisation by applying lime before emitting to the atmosphere.

The utilities area (Area H) is responsible for the cooling tower system, clean-in-place system and plant air system. Feedstock, chemicals, and products are stored in the storage area (Area F).

**2.3.2.2. Inventory data.** The mass balance, material consumption and atmospheric emissions for the five cases are summarised in Table 3. The emissions to air mainly occur in fermentation, WWT and combustion processes. The amount of  $CO_2$  emitted from fermentation, the open-top aerobic digester, and combustor is derived from the process simulation. The fugitive loss of methane from anaerobic digestion is estimated as 3% [39]. The emissions for

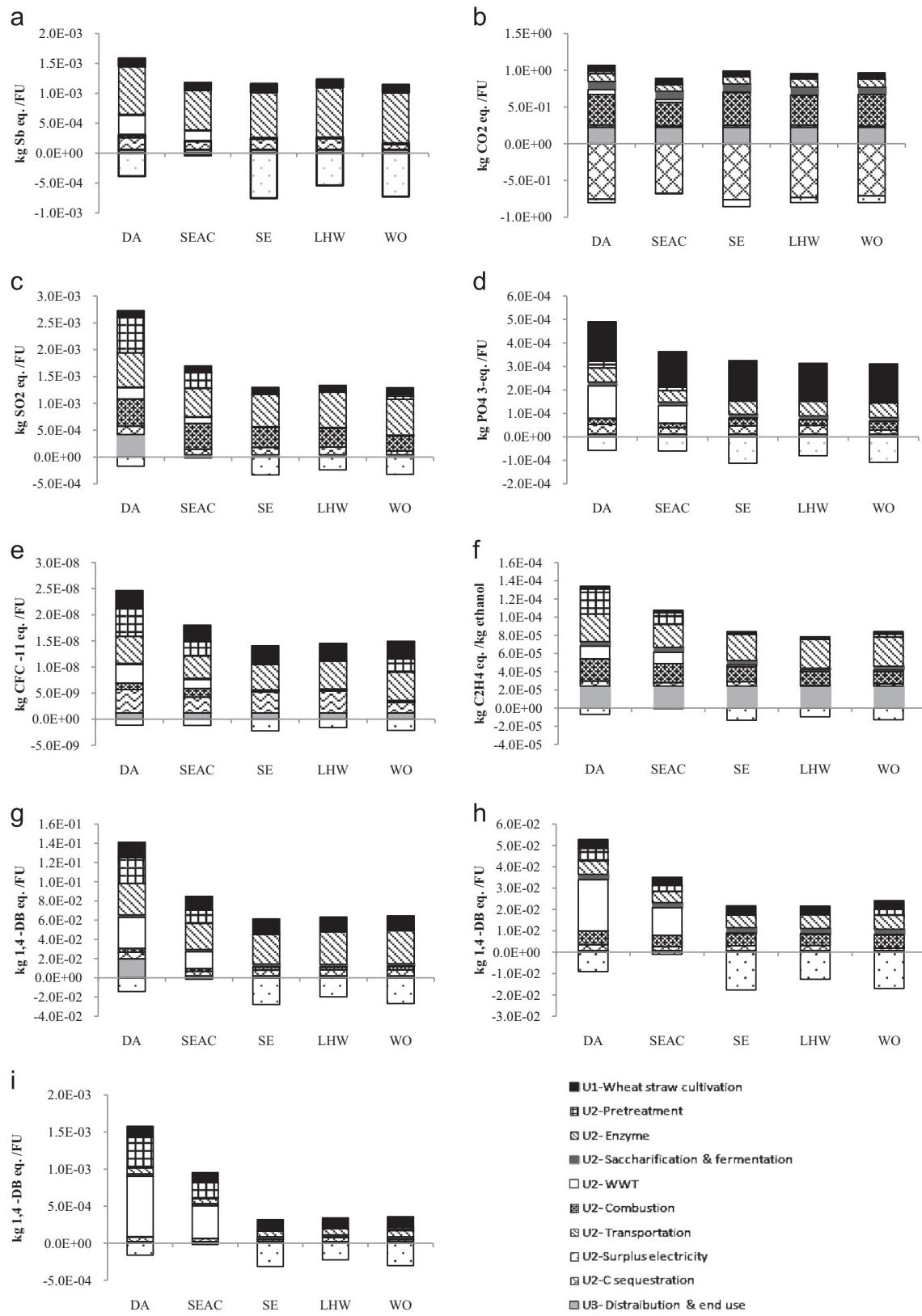
carbon monoxide (CO) and nitrogen oxides ( $NO_x$ ) were estimated based on the heating value of the combustion feed stream and the emission factor 0.31 kg/MWh, adopted from the NREL study [36]. Sulphate ions introduced into processes operating with acid (i.e. SEAC and DA) present problems for WWT. Therefore, lime is required to precipitate the sulphur in the WWT feed stream to control the sulphate concentration such that it is within the design limit of 4.4 g/L [36]. All Sulphur in feedstock and WWT streams are assumed to be completely converted into hydrogen sulphide ( $H_2S$ ) and oxidised into sulphur dioxide ( $SO_2$ ) during combustion. 1% of  $SO_2$  is also assumed to become sulphuric acid ( $H_2SO_4$ ). In processes where acid is used in the pretreatment, lime is applied to reduce  $SO_2$  emissions. The resulted gypsum and combustion bottom ash are modelled to landfill disposal.

The inventory data for enzyme (Cellic Ctec) production are provided by Novozymes A/S Denmark. Data for other chemicals, nutrients, waste treatment operation (e.g. landfill), infrastructure and National Grid electricity (UK-based average) are adopted from the Ecoinvent v2.2 database research reports [32,40,41].

The wheat straw is assumed to be transported from farmland to the bioethanol plant for a distance of 100 km by diesel lorry (> 28 t). Chemicals, fertiliser and nutrients are delivered by train for 100 km followed by diesel lorry for 150 km (20–28 t). In addition to that, enzymes transportation also includes 800 km by ship.

### 2.3.3. Bioethanol system unit process—U3 bioethanol distribution and end use

The bioethanol produced is assumed to be transferred from the plant to storage for a distance of 150 km by diesel lorry (20–28 t) and is then distributed to forecourt for another 150 km. Infrastructure, water and electricity use in storage were included from Jungbluth's report [40]. The  $CO_2$  emissions from bioethanol combustion in the FFV were estimated theoretically by assuming all carbon in bioethanol is converted to  $CO_2$ .



**Fig. 4.** Contribution analysis of environmental profile for bioethanol (unit: 'to drive 1 km'). (a) ADP, (b) GWP<sub>100</sub>, (c) AP, (d) EP, (e) ODP, (f) POCP, (g) HTP, (h) FATEP and (i) TEP.

#### 2.3.4. Petrol system

The inventory data for low sulphur petrol production and combustion were adopted from Ecoinvent v2.2 research reports [42,43].

#### 2.4. Allocation method

Allocation, required for allocating environmental burdens between multi-products is one of most critical issues in LCA

**Table 4**

LCA results for different wheat straw bioethanol pathways.

| Impact category                               | DA       | SEAC     | SE       | LHW      | WO       |
|---|----------|----------|----------|----------|----------|
| ADP, kg Sb eq./FU <sup>a</sup>                | 1.19E–03 | 1.13E–03 | 3.96E–04 | 6.85E–04 | 4.10E–04 |
| GWP <sub>100</sub> , kg CO <sub>2</sub> /FU   | 0.264    | 0.212    | 0.134    | 0.156    | 0.166    |
| AP, kg SO <sub>2</sub> eq./FU                 | 2.18E–03 | 1.68E–03 | 9.63E–04 | 1.09E–03 | 9.67E–04 |
| EP, kg PO <sub>4</sub> eq./FU                 | 4.33E–04 | 3.03E–04 | 2.12E–04 | 2.33E–04 | 2.02E–04 |
| ODP, kg CFC-11 eq./FU                         | 2.35E–08 | 1.68E–08 | 1.19E–08 | 1.29E–08 | 1.28E–08 |
| POCP, kg C <sub>2</sub> H <sub>4</sub> eq./FU | 1.27E–04 | 1.07E–04 | 7.09E–05 | 6.88E–05 | 7.14E–05 |
| HTP, kg 1,4-DB eq./FU                         | 1.09E–01 | 8.33E–02 | 3.36E–02 | 4.34E–02 | 3.76E–02 |
| FATEP, kg 1,4-DB eq./FU                       | 4.22E–02 | 3.72E–02 | 2.49E–03 | 7.47E–03 | 5.68E–03 |
| TEP, kg 1,4-DB eq./FU                         | 1.42E–03 | 9.36E–04 | 5.81E–06 | 1.17E–04 | 5.56E–05 |

<sup>a</sup> FU=function unit, 'to drive 1 km in a Flexible-fuel vehicle (FFV)'.

methodology. In our study, the multi-output processes are: (1) agricultural production where both wheat grain and straw are produced; and (2) bioethanol production where both ethanol and electricity are produced. In the baseline scenario, environmental burdens associated with wheat cultivation are allocated between wheat grain and wheat straw based on their economic values while burdens associated with additional fertiliser use and soil carbon change are assigned to wheat straw only in the sensitivity analysis scenario. In addition, 'system expansion' was applied on surplus electricity which is credited with avoided emissions from generation of an equivalent amount of the average UK National Grid electricity.

## 2.5. Characterisation model and impact categories

Characterisation model CML baseline 2000 v2.05 incorporated in SimaPro v7.3 was used to conduct the Life Cycle Impact Assessment (LCIA). The impact categories considered are Abiotic resources Depletion Potential (ADP), Acidification Potential (AP), Eutrophication Potential (EP), Global Warming Potential (100 year horizon) (GWP<sub>100</sub>), Ozone layer Depletion Potential (ODP), Human Toxicity Potential (HTP), Freshwater Aquatic Ecotoxicity Potential (FAETP), Terrestrial Ecotoxicity Potential (TEP) and Photochemical-Oxidants Creation Potential (POCP). These impact categories are explained in Section 3.

## 2.6. Sensitivity analysis

To study how and to what extent the wheat straw removal could influence the environmental profiles of bioethanol and its comparison results with petrol, a 'wheat straw removal' scenario is conducted here to compare with the baseline scenario where these effects are not considered.

The main environmental impacts related to the removal of wheat straw include the requirement of additional fertiliser to balance the nutrients removed with wheat straw, the change in soil organic carbon and the decrease in field emissions from wheat straw [19].

Concerning the additional fertilisers, environmental burdens regarding their production and their use due to field emissions (i.e. CH<sub>4</sub> and N<sub>2</sub>O) are added to the wheat straw cultivation process. These environmental burdens are shown as EB<sub>fertiliser production</sub> and E<sub>fertiliser use</sub> in the following equation. It should be noted that the wheat straw removed is supposed to otherwise have degraded in the field. Therefore, this removal decreases the amount of wheat straw left and reduces the consequent N<sub>2</sub>O emissions. This reduction is presented as N<sub>2</sub>O<sub>removed straw</sub>.

The removal of wheat straw can also lead to a loss of soil carbon which is emitted as CO<sub>2</sub> that is presented as ΔSOC in the equation. It was reported that the soil carbon loss due to wheat straw removal is 0.275 t C/ha in 20 per years (13.75 kg C/ha/year) and

used in this study [19]. However, the change in soil carbon is highly dependent on soil type, climate conditions and field operations etc. To obtain data in better quality may be of interest for the further research.

$$\Delta EB = EB_{fertiliser\ production} + E_{fertiliser\ use} - N_2O_{removed\ straw} + \Delta SOC$$

## 3. Results and discussion

### 3.1. Contribution analysis of LCA results for bioethanol

In this section, results for 'well-to-wheel' analysis on bioethanol produced from wheat straw using five different pretreatments are compared in Fig. 4 and the overall net LCA results for each impact category are presented in Table 4. In Fig. 4, the 'above-the-line' scores represent environmental burdens, whilst 'below-the-line' scores represent environmental savings (i.e. carbon sequestered in wheat straw and the avoided emission credits from the surplus electricity).

#### 3.1.1. Abiotic resources depletion potential (ADP)

ADP (kg Sb eq.), referring to the decrease of non-living natural resources (including energy resources) such as minerals or crude oil, is a very widely used impact category reflecting fossil fuel energy use. It is shown in Fig. 4(a) that the enzyme production is the dominant contributor to ADP in all five cases ranging from 50% to 80%. This is because enzyme production is an energy intensive process, with consumption mainly of natural gas. A significant amount of surplus electricity (25.8 MW) is obtained from bioethanol production using steam explosion (SE) pretreatment. Therefore, the considerable credits obtained by replacing national grid electricity offset its environmental burdens and gives the lowest overall ADP score.

#### 3.1.2. Global warming potential (GWP<sub>100</sub>)

In Fig. 4 (b), the green 'below-the-line' score accounts for the C sequestration in wheat straw and other inputs containing biogenic carbon. This score offsets CO<sub>2</sub> emissions derived from biogenic carbon in combustion, saccharification & fermentation and ethanol end use processes. Therefore the net overall GHG emissions per functional unit are 0.26 kg CO<sub>2</sub> eq. for DA, 0.21 kg CO<sub>2</sub> eq. for SEAC, 0.13 kg CO<sub>2</sub> eq. for SE, 0.16 kg CO<sub>2</sub> eq. for LHW, and 0.17 kg CO<sub>2</sub> eq. for WO pathway (see Table 4). Wheat straw cultivation contributes between 30% and 60% to the net GHG emissions, which is due to N<sub>2</sub>O emission by applying fertiliser. Another 40%–60% of the overall net score is accounted for by enzyme production which is a highly energy intensive process. Production of sulphuric acid and ammonia used in DA and SEAC pretreatment are the main contributors to burdens in the pretreatment process.

### 3.1.3. Acidic potential (AP)

Enzyme production is found to be the dominant contributor to the overall burdens due to SO<sub>2</sub> emissions from fossil fuel consumption. In DA and SEAC pathways, the production of sulphuric acid is the main contributor to the pretreatment process, accounting for 86% and 81% respectively. In the combustion process, the sulphur contained in wheat straw feedstock and other inputs is converted to SO<sub>2</sub> and accounts for 23–40% of the overall net score. The burdens in wheat straw cultivation are mainly caused by the field operation emissions from diesel consumption.

### 3.1.4. Eutrophication potential (EP)

Eutrophication potential is generally associated with the environmental impacts of excessively high nutrients (i.e. N and P) that lead to shifts in species composition and increased biological productivity (e.g. algal blooms) [44]. In Fig. 4(d), the wheat straw cultivation process is the dominant contributor to the 'above-the-line' score. In this process, N<sub>2</sub>O emissions contribute to over 60%, while wheat seed production accounts for around 20% of burdens and the rest is from fertiliser production. For DA and SEAC pathways, the burdens for WWT are due to the production of sodium hydroxide (NaOH) that is used to neutralise nitric acid (HNO<sub>3</sub>) as a result of ammonia neutralising acid during pretreatment.

### 3.1.5. Ozone layer depletion potential (ODP)

ODP, referring to the decrease in the total volume of ozone in the Earth's stratosphere, is caused by various chlorinated and bromated substances [25]. In addition to enzyme production (shown in Fig. 4(e)), wheat straw cultivation causes considerable burdens caused by pesticide production (40%) and fertiliser production (50%). In DA and SEAC pathways, ammonia production contributes to over 90% of the burdens in pretreatment.

### 3.1.6. Photochemical-oxidants creation potential (POCP)

The photochemical oxidation, also referred as summer smog, is the result of reactions between NO<sub>x</sub> and hydrocarbons or volatile organic compounds (VOC) [44]. In Fig. 4(f), burdens in enzyme production are due to emissions from fossil fuel consumption while those in combustion are due to SO<sub>2</sub> emissions. In the 'Distribution & end use' module, the fugitive ethanol emissions (0.5 g/kg fuel) in ethanol storage account for 30% of its burdens, whilst CO and SO<sub>2</sub> emissions in ethanol distribution are responsible for the remainder.

### 3.1.7. Ecotoxicity (Human toxicity potential—HTP, freshwater aquatic ecotoxicity potential—FAETP, terrestrial ecotoxicity potential—TEP)

In DA and SEAC pathways where acid is used in pretreatment, WWT is the biggest contributor to all toxicity categories due to the production of NaOH which is used in WWT (Fig. 4(g), (h) and (i)). For HTP and TEP, burdens in pretreatment are due to acid production while those in wheat straw cultivation are because of pesticide production. For FAETP, NO<sub>x</sub> emissions from landfill of bottom ash are the main cause.

In SE, LHW and WO pathways, enzyme production is the dominant contributor to HTP and FAETP while wheat straw cultivation contributes most to TEP. The credits from surplus electricity offset the 'above-the-line' burdens considerably, resulting in relatively low net burdens for these three pathways.

## 3.2. Comparison with petrol

The prospective scenarios of five pathways with different pretreatment methods are compared with petrol in Fig. 5. It is shown that wheat straw ethanol produced with SE, LHW and WO pretreatment methods are overall favourable over petrol,

particularly in ADP, GWP<sub>100</sub>, ODP, ecotoxicity and POCP impacts. The pathway with SEAC pretreatment is environmentally similar to petrol but delivers advantages in ADP, GWP<sub>100</sub>, ODP and HTP impacts. In contrast, bioethanol production using DA pretreatment is less favourable over petrol in most impact categories. In general, DA and SEAC pathways result in higher impacts (i.e. ADP, toxicities, GWP<sub>100</sub> and POCP) than other pretreatments because of the use of acid and sodium hydroxide. For AP and EP, higher environmental burdens from bioethanol pathways than petrol are due to the combustion emissions in the CHP process and the utilisation of fertilisers in the agricultural process, respectively. Overall, it can be concluded that by replacing petrol with wheat straw bioethanol using the pretreatment methods studied here, with exception for DA pretreatment, savings of 11–45% in GHG emissions and 13–75% in abiotic resources depletion potential can be achieved. However, as discussed in Section 1, using wheat straw to produce ethanol instead of ploughing back into the field may cause consequential effects on the LCA comparison results with petrol; these are discussed in the sensitivity analysis.

### 3.3. Sensitivity analysis—system boundary

By including within the system boundary (1) the production and use of additional fertilisers required to compensate the removed wheat straw and (2) soil carbon change, bioethanol is compared with petrol (Fig. 6). It is shown that the rankings of five bioethanol pathways remain unchanged, while their comparison results with petrol are altered, particularly in GWP<sub>100</sub>, FATEP and TEP impact categories. Fertiliser production is a fossil fuel intensive process and therefore the additional requirement of fertiliser

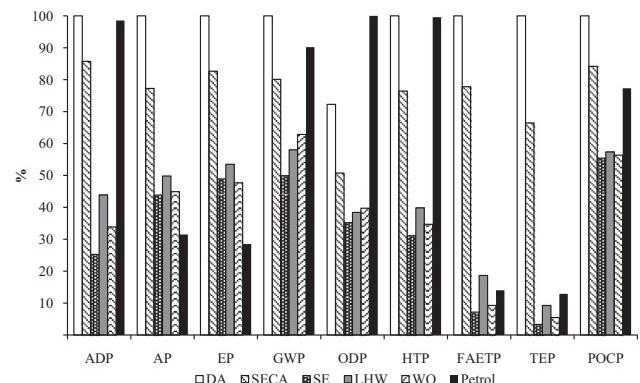


Fig. 5. Characterised LCIA comparison results for bioethanol (prospective scenarios for five cases) with petrol (unit: 'to drive 1 km in FFV').

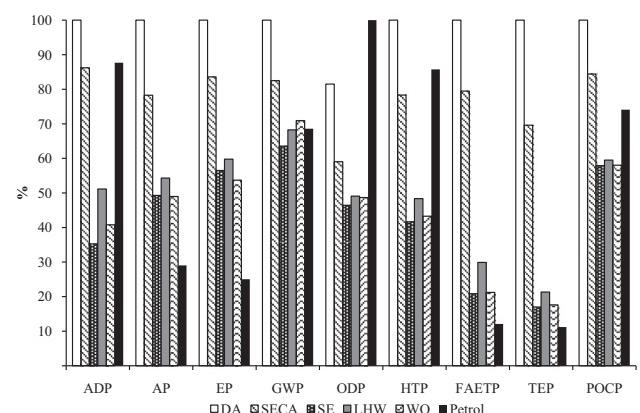


Fig. 6. Sensitivity analysis on system boundary—characterised LCIA comparison results for bioethanol with petrol (unit: 'to drive 1 km in FFV').

increases burdens in ADP, FAETP and TEP significantly. In addition, the increased field emissions caused by using this additional fertiliser are reflected in EP and GWP<sub>100</sub> score. Furthermore, CO<sub>2</sub> emissions from the lost soil carbon caused by wheat straw removal enlarge the GWP<sub>100</sub> score. Compared with the baseline scenarios (Fig. 5), wheat straw production with SE, LHW, WO pretreatment continues to have a better environmental performance than petrol, while SECA pretreatment is worse than petrol but still has advantages in ADP, ODP and HTP impact categories. For GWP<sub>100</sub> and ADP, wheat straw bioethanol can save only up to 25% and 60% respectively in GHG emissions and abiotic resources depletion potential compared to petrol even by considering the consequential effects of removing wheat straw from the field.

These findings suggest that the consequential effects of wheat straw removal including the additional requirement of fertiliser to compensate nutrient loss and CO<sub>2</sub> emissions due to soil carbon loss are not negligible in assessing the environmental impacts of a wheat straw to bioethanol life cycle. It is suggested that when wheat straw is used for producing ethanol, attention must be paid to develop the best management practices and to ensure enough straw is left in the field to maintain soil quality and productivity.

#### 4. Conclusions

This study presents a UK-based life cycle assessment on bioethanol production from wheat straw using current and emerging pretreatment technologies (i.e. dilute acid, steam explosion with and without catalyst, liquid hot water and wet oxidation) and evaluates their advantages and disadvantages from an environmental point of view. The contribution analysis for the near-term scenarios of bioethanol production indicates that enzyme production is a significant contributor to most of the impact categories, whilst wheat straw cultivation also contributes considerably to global warming, eutrophication and eco-toxicity potentials. These five wheat straw-to-bioethanol cases are further compared with conventional petrol, from which it is found that the pathways with steam explosion, liquid hot water and wet oxidation pretreatment are environmentally favourable over petrol. Overall, the ethanol production from wheat straw shows great potential to replace petrol by saving GHG emissions of up to 45% and fossil fuel usage of up to 75%. However, these conclusions are affected by the definition of the ethanol system boundary, which may or may not include the consequences of wheat straw removal. By considering these consequent effects, burdens for most impact categories are increased considerably, though certain ethanol pathway (i.e. steam explosion) still remains environmentally favourable over petrol.

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